2-Chloro-6-fluorobenzyl alcohol, 2-methylbutyl ether

Inchi: InChI=1S/C12H16ClFO/c1-3-9(2)7-15-8-10-11(13)5-4-6-12(10)14/h4-6,9H,3,7-8H2,1-2H3

InchiKey: NSDBQBIKKFKGQJ-UHFFFAOYSA-N

Formula: C12H16ClFO

SMILES: CCC(C)COCc1c(F)cccc1Cl

Mol. weight [g/mol]: 230.71

Physical Properties

Property code	Value	Unit	Source
gf	-170.87	kJ/mol	Joback Method
hf	-426.77	kJ/mol	Joback Method
hfus	25.04	kJ/mol	Joback Method
hvap	51.50	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	4.042		Crippen Method
mcvol	176.060	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	1462.00		NIST Webbook
rinpol	1462.00		NIST Webbook
tb	569.28	K	Joback Method
tc	768.24	K	Joback Method
tf	314.20	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.74	J/mol×K	569.28	Joback Method
cpg	425.41	J/mol×K	602.44	Joback Method
cpg	439.35	J/mol×K	635.60	Joback Method
cpg	452.57	J/mol×K	668.76	Joback Method
cpg	465.08	J/mol×K	701.92	Joback Method
cpg	476.90	J/mol×K	735.08	Joback Method
cpg	488.04	J/mol×K	768.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume